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# Size exclusion effect in binary inclusion compounds of α-cyclodextrin

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## Abstract

© 2018 the Owner Societies. The size exclusion of guests by α-cyclodextrin (aCD) in binary host-guest systems was observed to be a key structure-property relationship for the choice of this host as a receptor. For this, vapor sorption isotherms of water and volatile organic compounds were determined using dry aCD, which show an inclusion threshold by sorbate activity corresponding to a phase transition of guest (or water) inclusion. These phase transitions were also characterized using X-ray powder diffractograms. The analysis of these data shows that interaction of aCD with water does not differ much from that with organic compounds that can be included by aCD without water and therefore are water-mimicking as such. The inclusion and hydration Gibbs energies and composition of the saturated host-guest clathrates were determined from sorption isotherms. The Gibbs energies of guest inclusion by solid aCD and its hydration characterize the guest-host and water-host affinity in the solid state. The correlation of the obtained inclusion parameters with that of guest size indicate the ban on the inclusion of volatile hydrophilic organic compounds with more than three carbon atoms and smaller molecules without hydrophilic groups. These data may be used for estimation of the relative ability of more hydrophobic guests to replace water and organic solvents in solid aCD. The observed inclusion of water and small hydrophilic molecules by solid aCD with phase transition gives an alternative insight into the role of water in activating the inclusion of more hydrophobic guests. Furthermore, the results show the extent to which aCD may be preferable in applications using water or other solvents.

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